Integrating Open Source Software Applications for Building Molecular Dynamics Systems

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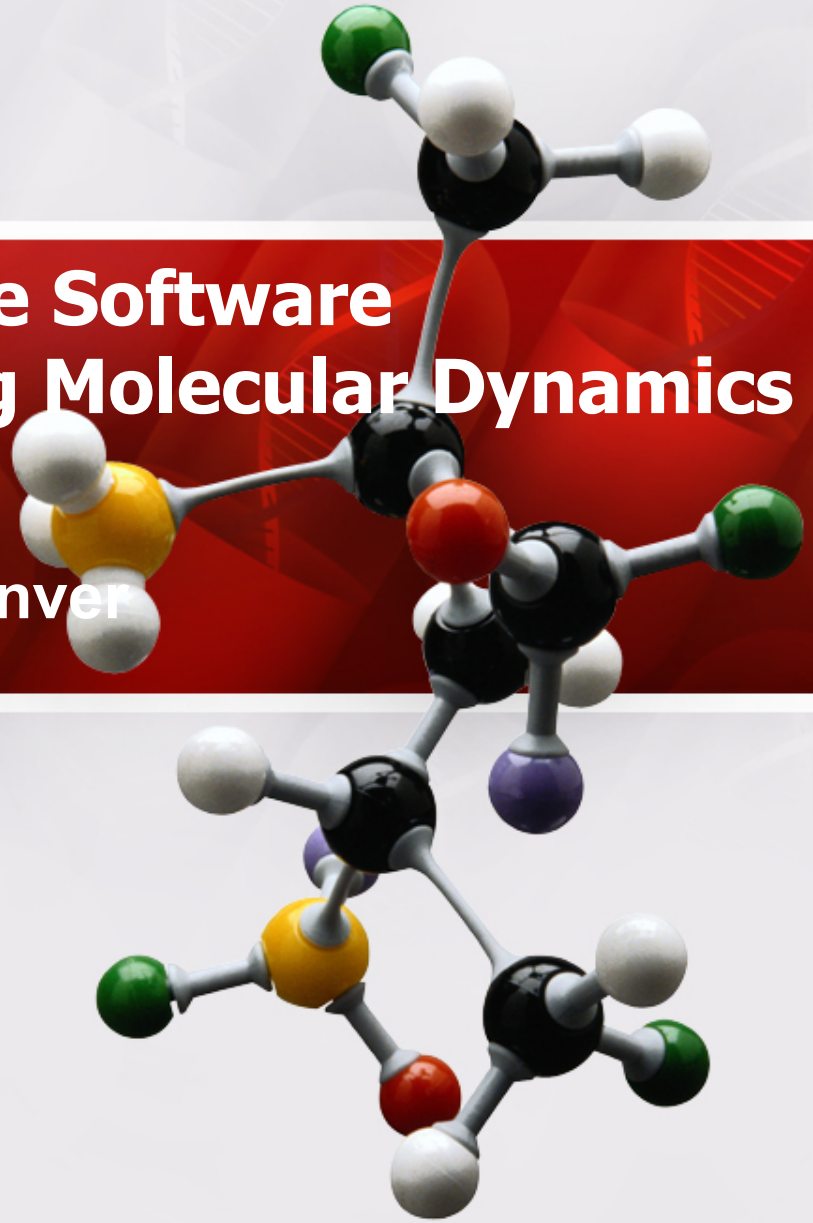
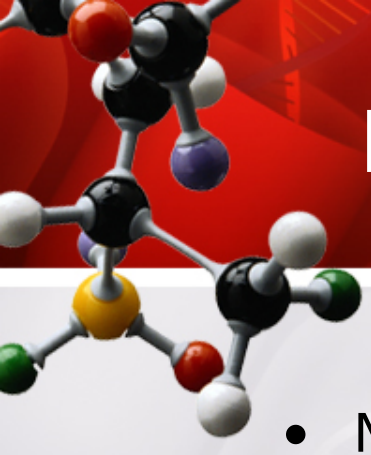


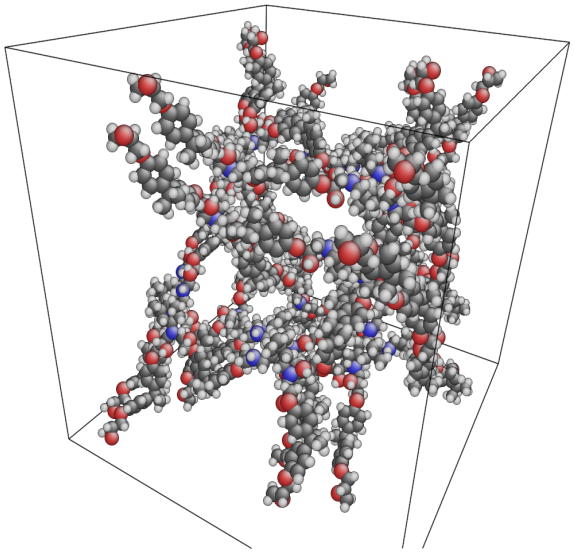


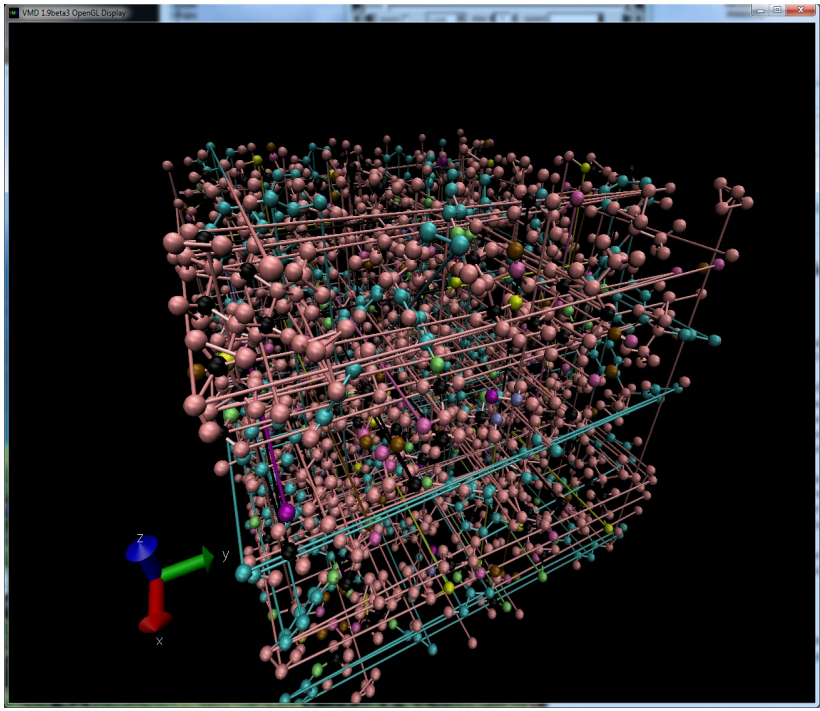
Problem Space

- Molecular Dynamics (MD) Simulations are hampered by long build times for an MD cell.
- Maintaining geometry in MS Excel
- Difficult to build different geometries
- MD cell creation may rely on one knowledgeable individual
- Anecdotal data above from other researchers
- If you pick the wrong approach easy stuff becomes hard

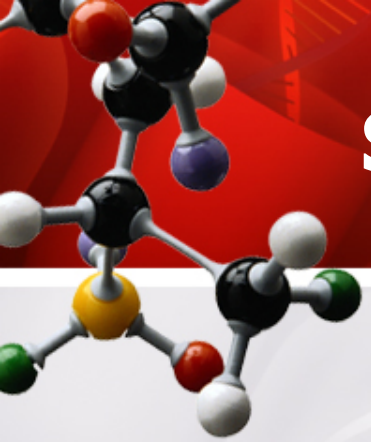
What is an MD Cell?

- A finite volume, usually a cube from 10Å to 100Å per side (small MD Cell)
- Contains all molecules for a simulation
- Comes in two varieties:
  - Initial (cell 55Å per side)
  - Final (cell 30-32Å per side)



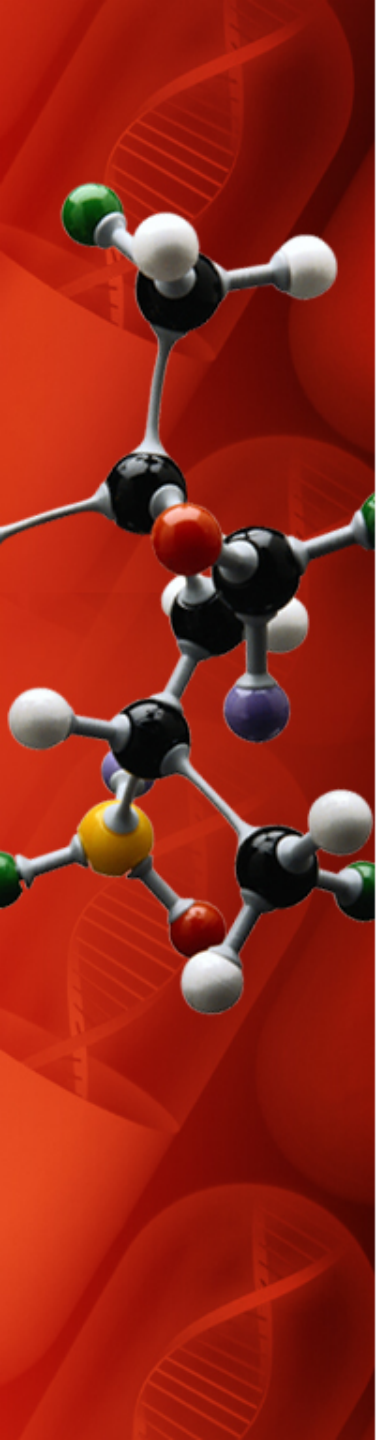


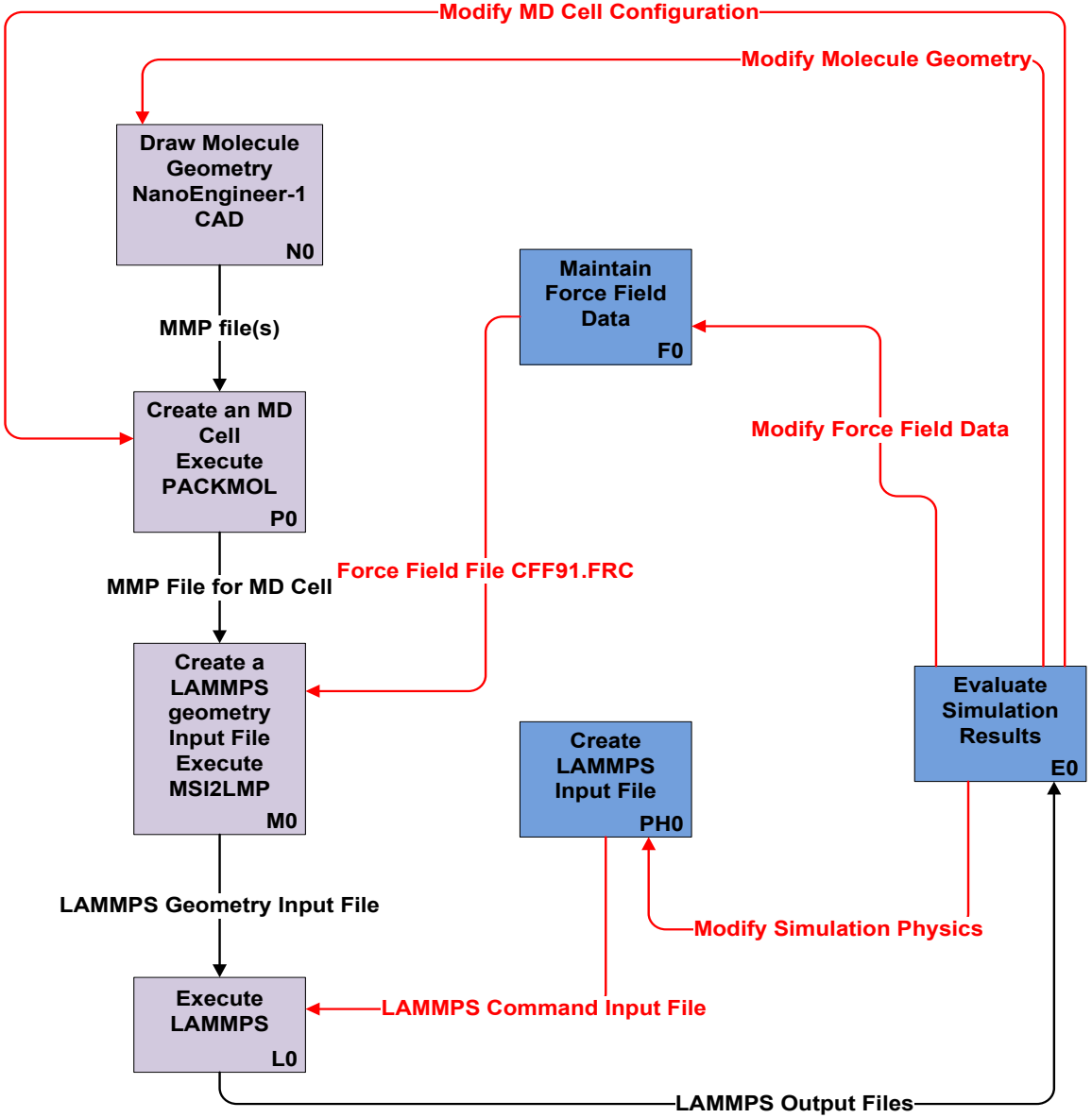
Solution Space



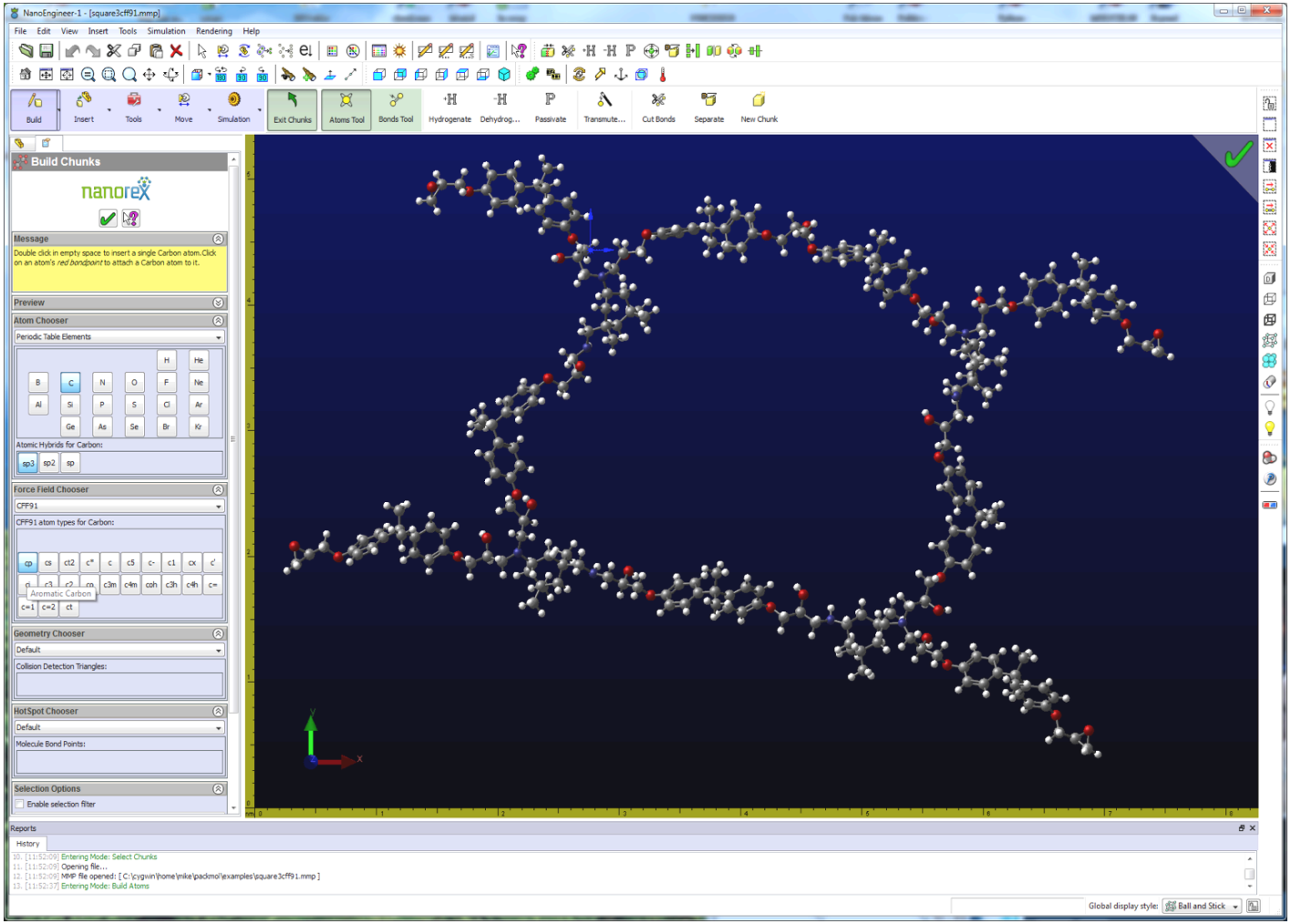
- Create a software by integrating existing open source software.
  - **Design geometric molecule models via CAD**
  - **Build an MD cell from the CAD molecule models**
  - **Generate a LAMMPS Geometry Input File (LGIF)**
- After careful analysis and lots of luck the following applications were chosen for integration
  - **NanoEngineer-1**
  - **Packmol**
  - **msi2lmp**

How the Programs Work Together



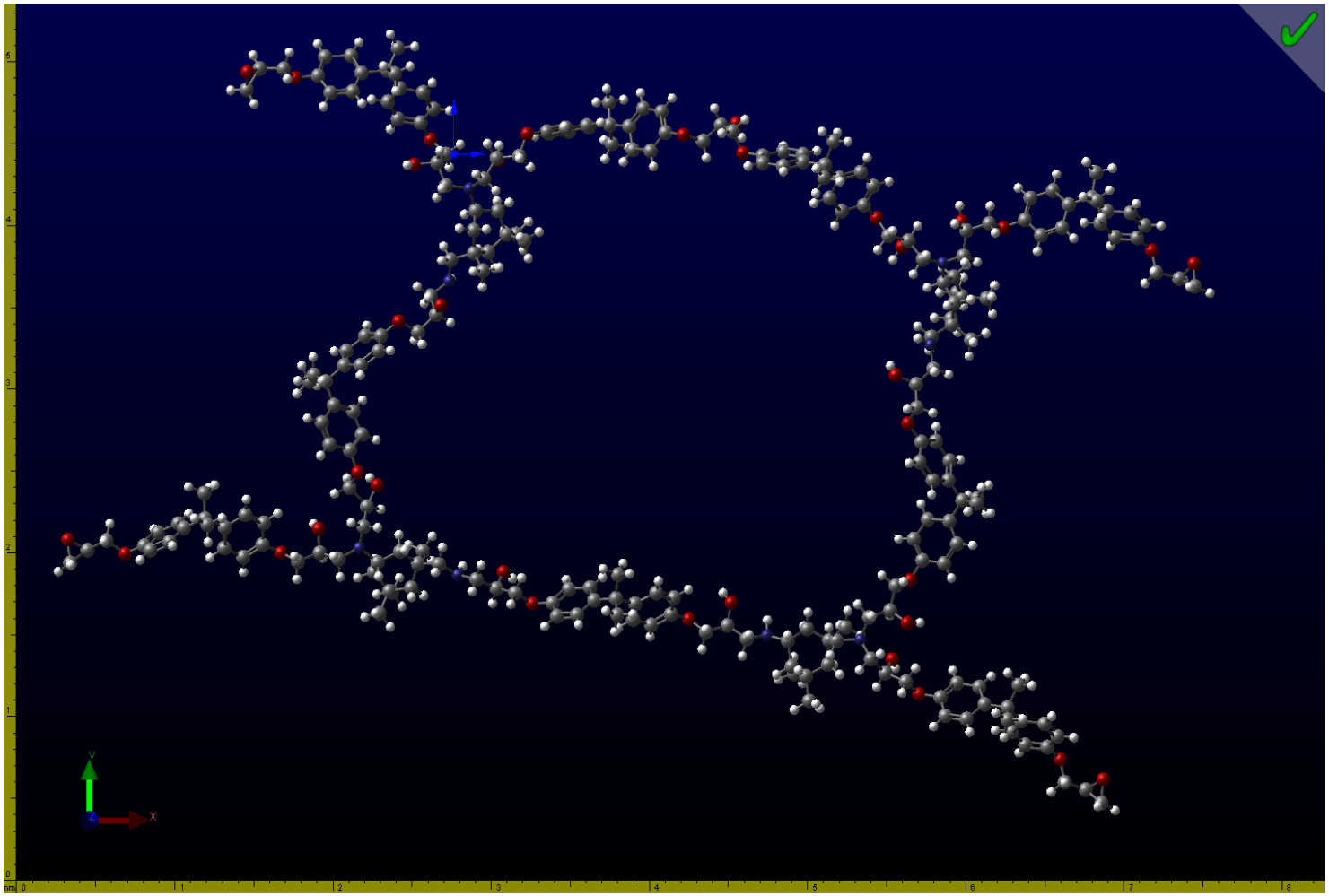


NanoEngineer-1 CAD Software



NanoEngineer-1 CAD Software

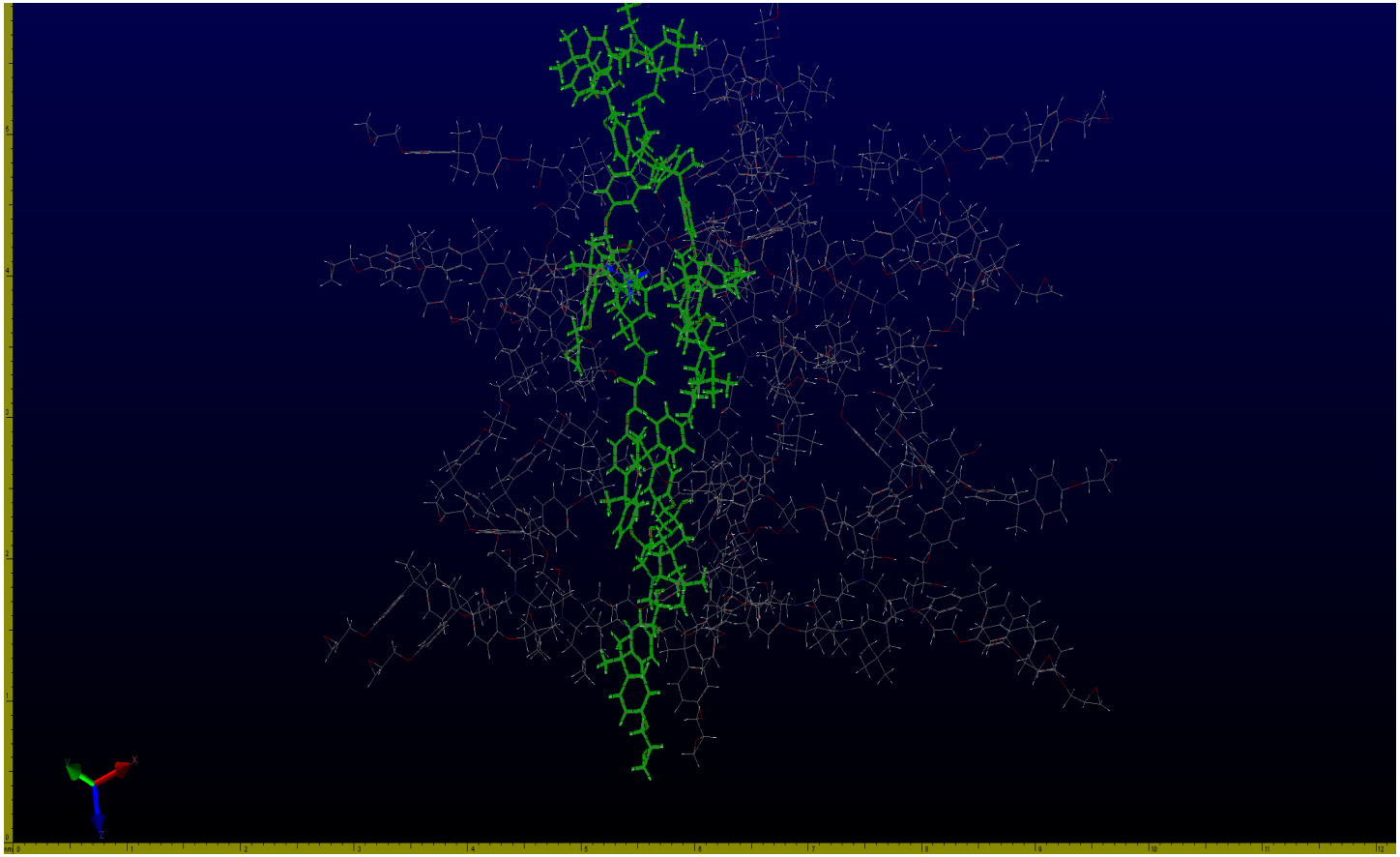
- Oligomer contains 569 atoms

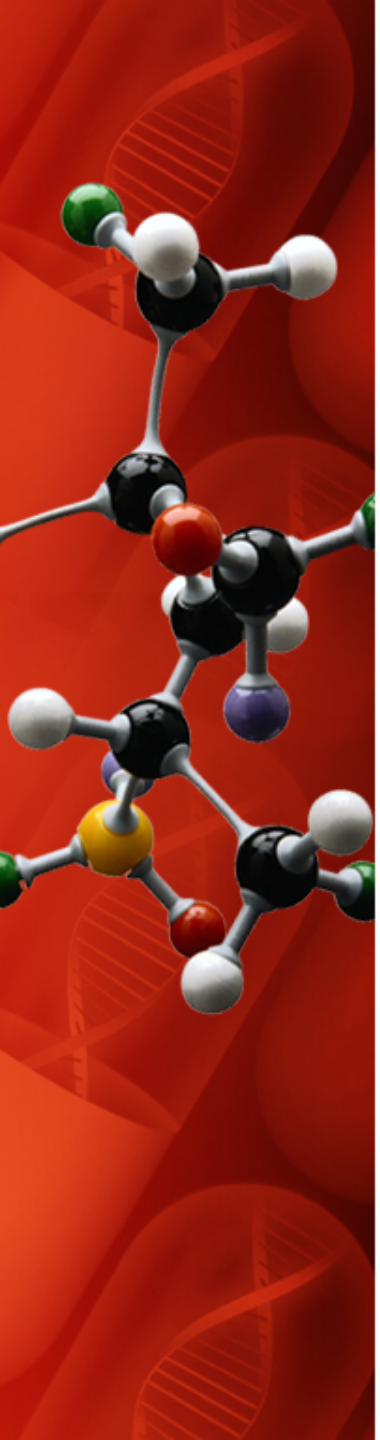


75% intra-crosslinked oligomer for constructing an MD cell

Packmol MD Cell

- Highlighted in green one oligomer in a system of five oligomers
- **Shows intertwined oligomers**
- Creates an MMP file – can be read/edited by NanoEngineer-1

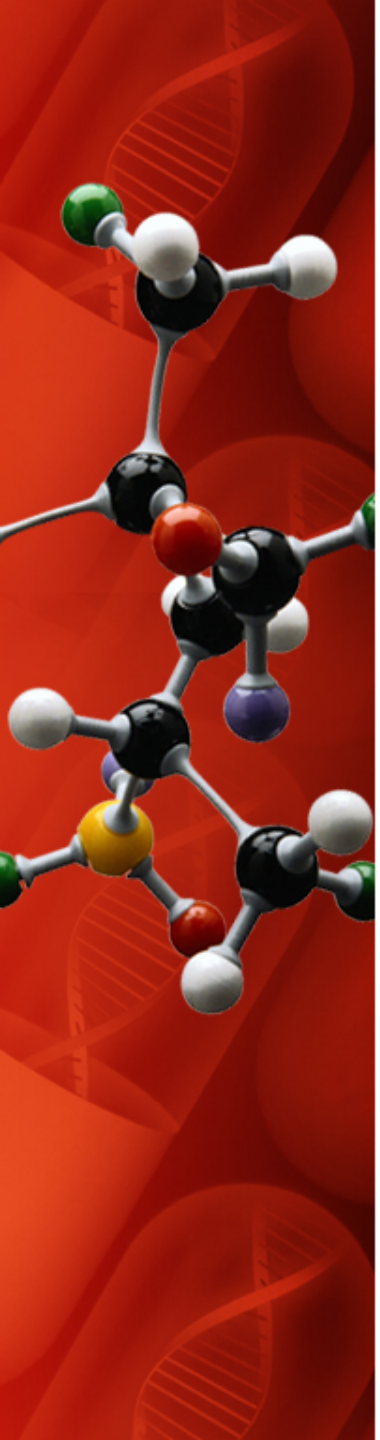


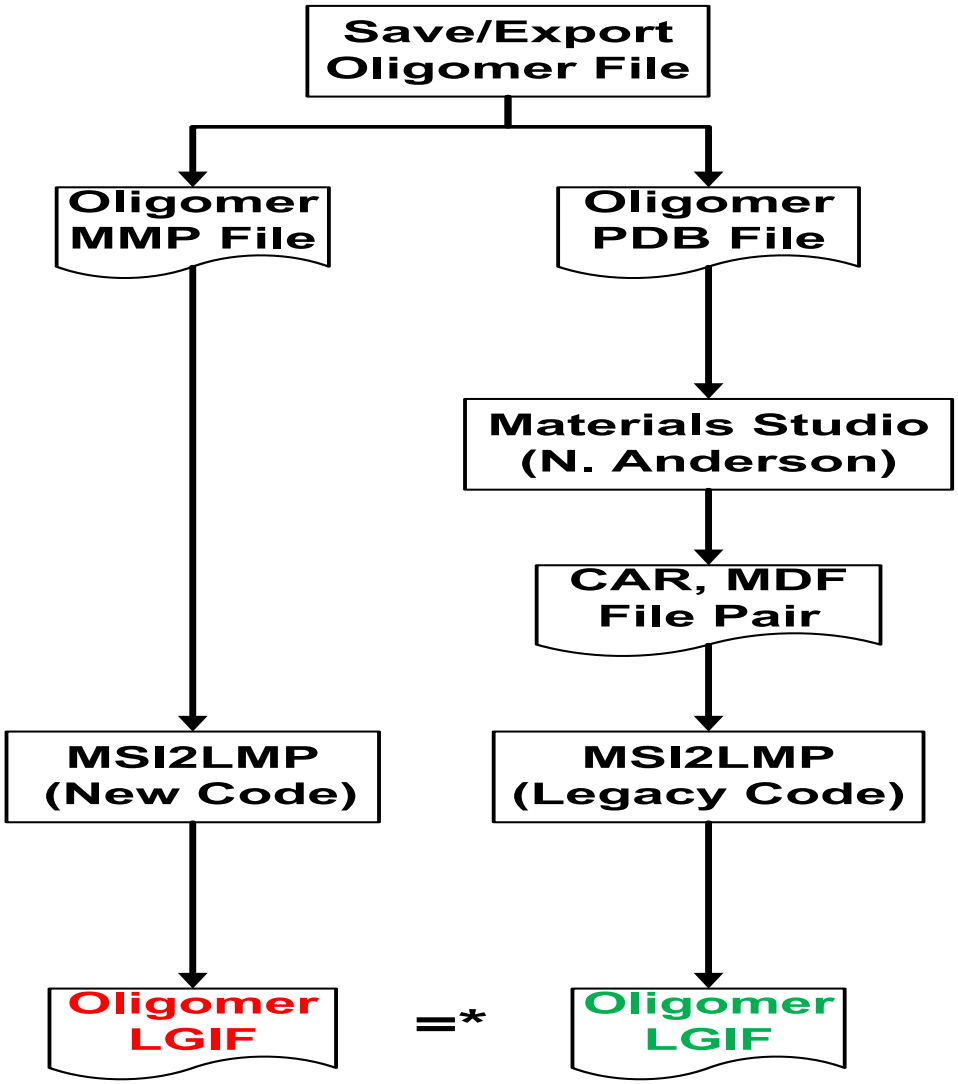


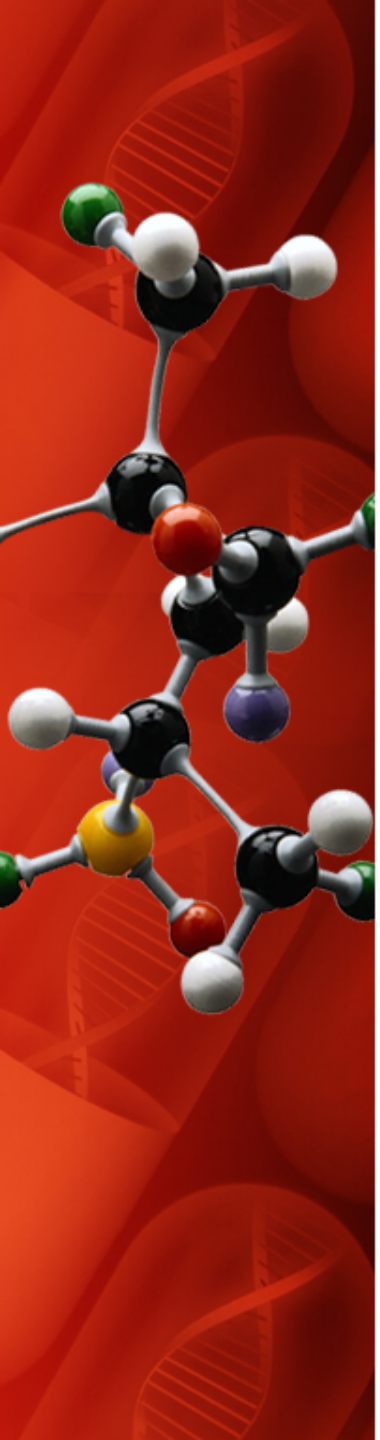
msi2lmp

- Now converts the Packmol MMP file into the LAMMPS Geometry Input File (LGIF)
- Monumental task done very quietly
- Most significant implementation went from $O(n^2)$ to $O(n \log n)$!!!

Software Parallel Testing (MSI2LMP)



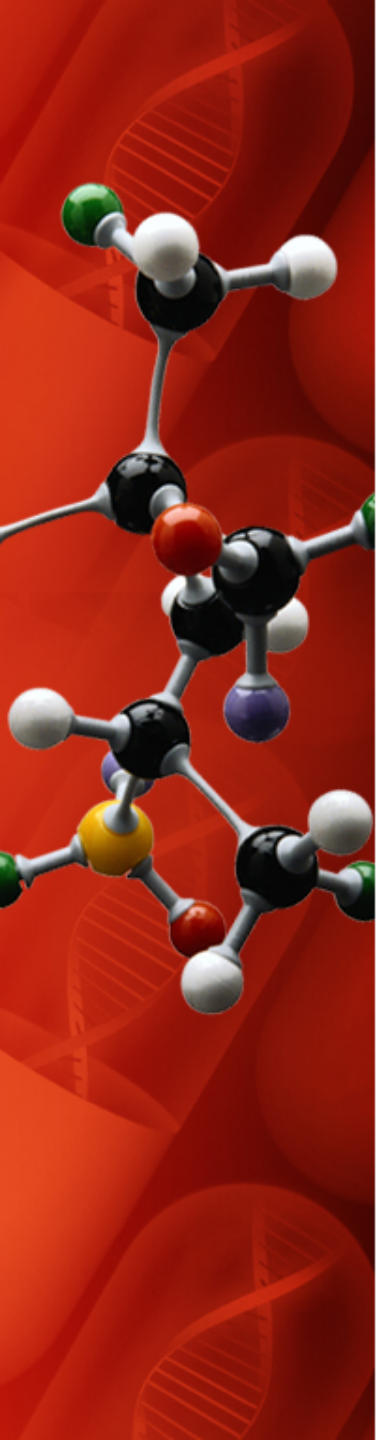




NanoEngineer-1 Software Testing

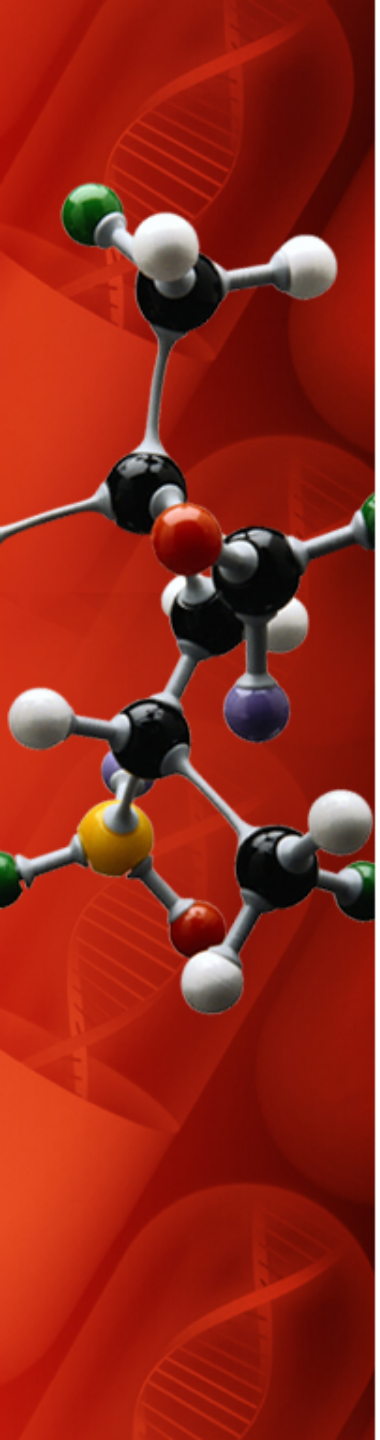
NanoEngineer-1 Software Feature	Test Method
Multiple Force Field Support	Atom types for CFF91 and COMPASS verified in GUI and in MMP file. The GUI force field Combo box allows a valid force field to be selected by the user.
Manual Atom typing	Atom types assigned in the GUI to atoms are written to the MMP file and read from the MMP file. Verification through ToolTips feature validates feature.
Collision detection*	Atoms are marked in threes by left-clicking in GUI – Triangle data is written to MMP file. GUI side bar displays a Triangle button for a created triangle. Triangle data is read from the MMP file and unhides triangle buttons in GUI.
HotSpot (crosslinker) *	**Two terminal atoms are highlighted via right-clicks to form a HotSpot. The first is male the second is female. A button is displayed in the GUI for the HotSpot. The HotSpot was successfully processed by SAW software to create long chain polymers from the DGEBA monomers.**
Delete Atom	When deleting an atom its triangle and hotspot attributes are checked and fixed. Triangles and HotSpots are deleted. The GUI is updated. Data written to the MMP file is written correctly.
Atom Selection	When selected in the GUI an atom will display a ToolTip balloon containing the chemical atom type and the numeric atom type.
Used WingIDE debugger	Visual inspection of variables and logical paths in software for above changes
ToolTip GUI Dialog	When created an atom must have a force field associated with it. The chemical and numeric force field is displayed in the tool tip balloon window. The ToolTip dialog box allows the user to turn the feature on and off. The Checkboxes were exercised and found to work as expected.

*Features added to support SAW



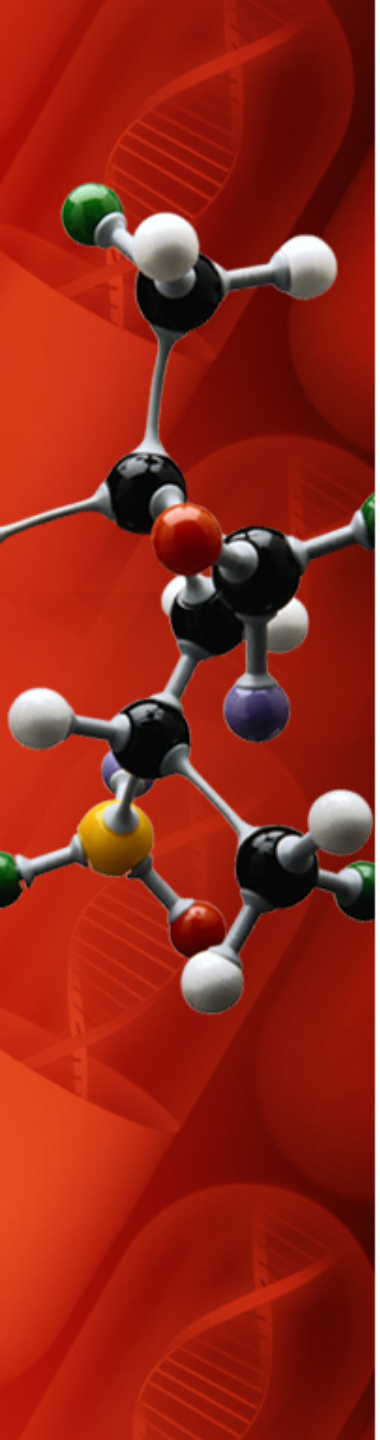
PACKMOL Software Testing

PACKMOL Software Feature	Test Method
Read MMP Files	Visually inspected data structures in core PACKMOL software to insure atom attribute data was populating spatial and force field variables in the software.
Write MMP Files	Visually inspected data structures containing the newly created molecules and compared the number of atoms per molecule and the number of molecules to the PACKMOL control file.
Used Dynamic Display Debugger (open source)	All FORTRAN code modified and written was visually inspected using the debugger



MSI2LMP Software Testing

MSI2LMP Software Feature	Test Method
Read MMP Files	Visually inspected data structures in core MSI2LMP software to insure atom attribute data was populating spatial and force field variables in the software.
Write LAMMPS Trajectory File	Used VMD software to display cell of molecules and compared atom numbers to numbers in MMP file.
Used Visual Studio	All C language code modified and written was visually inspected using the debugger
Molecule identification	Visually inspected LAMMPS Geometry Input File and data structures to insure that every unique molecule created could be identified in LAMMPS.
Numeric Force Field Feature	Visually verified that the number of parameters in the modified force field files were being correctly read in and stored for use by the parameterization function in the software.
Atom numbers, atom types, number of bonds, angles, dihedrals and impropers	These were cross checked by inspection between the MMP and the LGIF file.

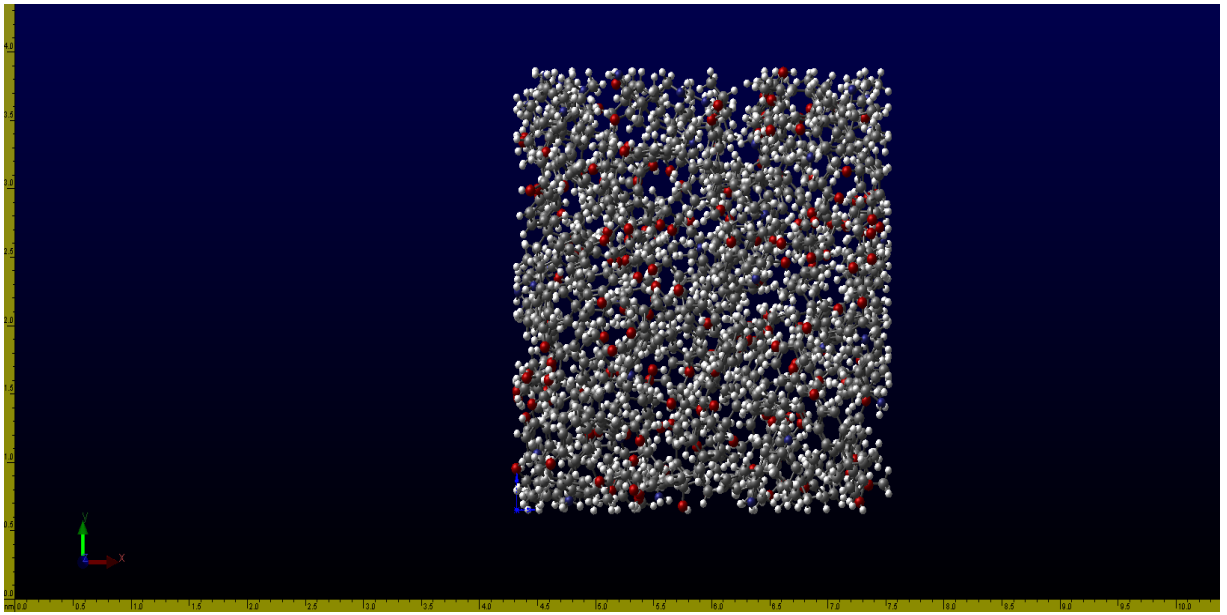


Software Quality/Reliability

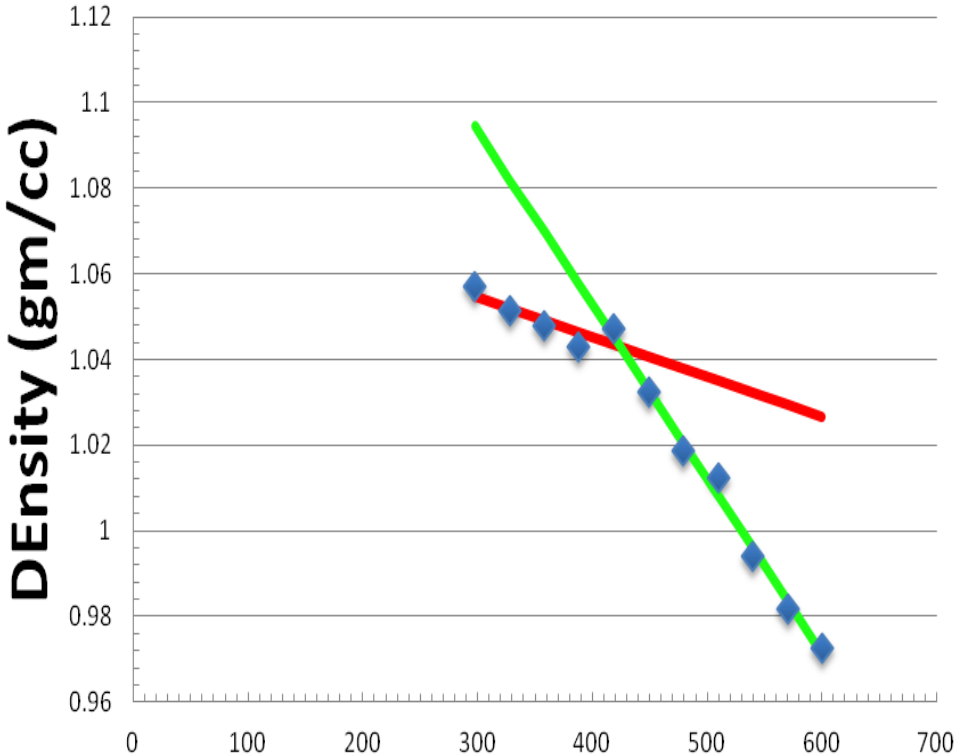
- Fixed many bugs so far
- The software is still a proof-of-concept with Alpha release Summer 2012
- Peers at DU are using software to create MD cells
- Minor bugs exist with work-a-rounds
- Continuing to fix bugs as they occur

System One (No Crosslinking)

- 45 DGEBA & 20 IPD molecules
- Density: ~1 gm/cc at 298K and 1atm
- Looks like the Borg Cube from Star Trek



System Two (75% Intra-crosslinked)



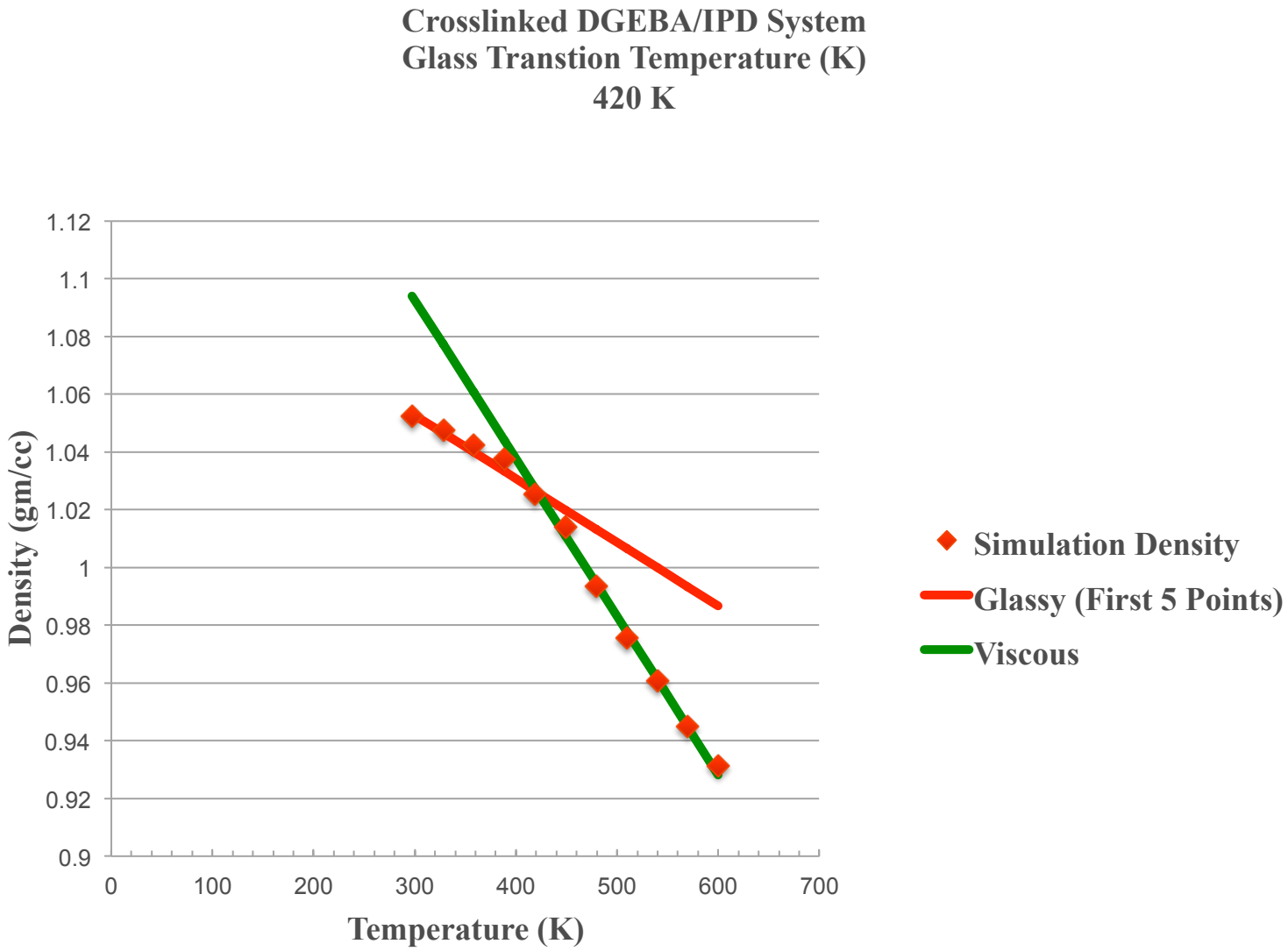
Crosslinked DGEBA/IPD System
Glass Transition Temperature (Tg)
423 K

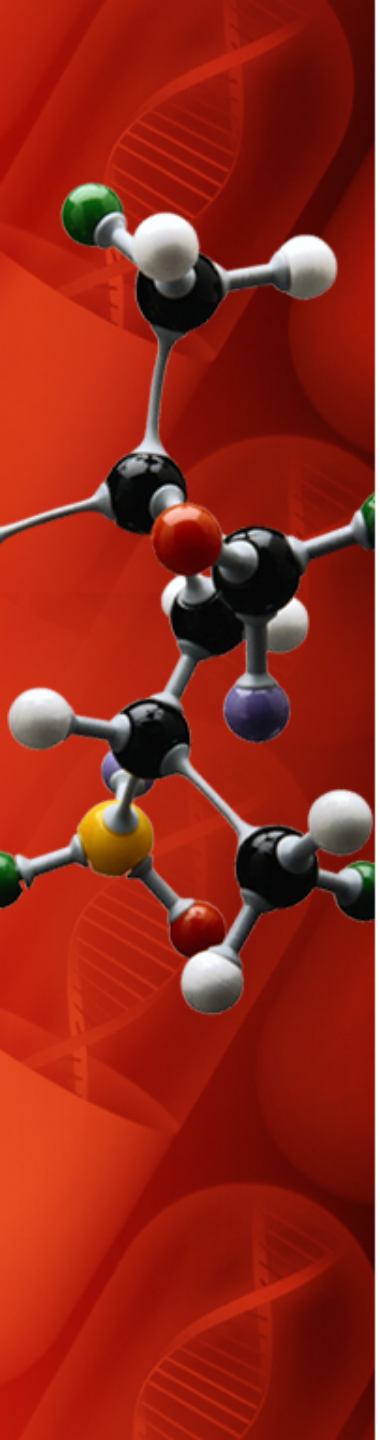
Simulation Density

Glassy (First 5 Points)

Viscous

System Three (87.5% Intra-crosslinked)





Simulation Results Summary

- Simulated Annealing creates the final MD cell, but at the expense of additional CPU time
- Acceptable results of MD simulations of density and glass transition temperature helps to validate software
- Crosslinking does increase density as shown by system one and two results and thereby increases the glass transition temperature